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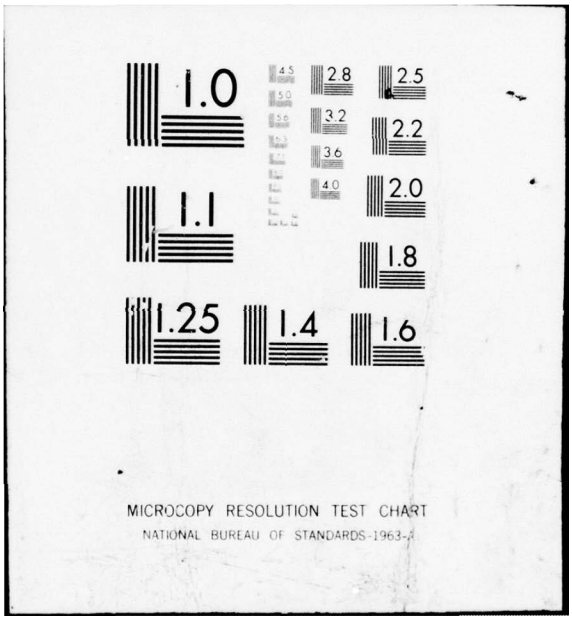
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FOURIER TRANSFORM INFRARED SPECTROSCOPY: DEMONSTRATION OF MEASUREMENT CAPABILITIES IN THE LABORATORY AND THE FIELD

January 1978

RESEARCH DEPARTMENT

GRUMMAN AEROSPACE CORPORATION
BETHPAGE NEW YORK

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SECURITY CLASSIFICATION OF THIS PAGE *(When Data Entered)*

REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER (14) RM-648	2. GOVT ACCESSION NO. / 3. RECIPIENT'S CATALOG NUMBER (9)
4. TITLE *(and Subtitle)* (6) Fourier Transform Infrared Spectroscopy: Demonstration of Measurement capabilities in the Laboratory and the Field.	5. TYPE OF REPORT & PERIOD COVERED Research memo
	6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) (10) Robert A. Reed	8. CONTRACT OR GRANT NUMBER(s)
9. PERFORMING ORGANIZATION NAME AND ADDRESS Grumman Aerospace Corporation So. Oyster Bay Road (Research Dept.) Bethpage, New York 11714	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS	12. REPORT DATE (11) Jan[redacted]78
	13. NUMBER OF PAGES ~~21~~ (12) 30 pp.
14. MONITORING AGENCY NAME & ADDRESS *(if different from Controlling Office)*	15. SECURITY CLASS. *(of this report)* Unclassified
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT *(of this Report)*

Approved for public release; distribution unlimited

17. DISTRIBUTION STATEMENT *(of the abstract entered in Block 20, if different from Report)*

18. SUPPLEMENTARY NOTES

19. KEY WORDS *(Continue on reverse side if necessary and identify by block number)*

Infrared, plume

20. ABSTRACT *(Continue on reverse side if necessary and identify by block number)*

The measurement capabilities of an infrared interferometer spectrometer are documented for both field and laboratory usage. This instrument provided intermediate resolution coverage (0.3 cm^{-1} to 5 cm^{-1}) in the 1.6 to 5.4 micron spectral interval. It has been used in the field to study radiation from aircraft exhaust plumes, background emission, and atmospheric transmission. In the laboratory, line spectra of flames have been measured and nonequilibrium vibrational temperatures derived. System configuration, operating procedure, and

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Grumman Research Department Memorandum RM-648

FOURIER TRANSFORM INFRARED SPECTROSCOPY: DEMONSTRATION OF MEASUREMENT CAPABILITIES IN THE LABORATORY AND THE FIELD

by

Robert A. Reed

Aerophysics

January 1978

Approved by: Richard A. Scheuing
Richard A. Scheuing
Director of Research

ACKNOWLEDGEMENTS

The author is indebted to M. W. Slack for guidance and support in all phases of the work reported herein. T. Hilgeman and L. Smith assisted with the data processing. R. Gundersen helped with the field measurements, and J. Bilenas provided helpful discussions concerning the Mohawk suppressor project.

ABSTRACT

The measurement capabilities of an infrared interferometer spectrometer are documented for both field and laboratory usage. This instrument provided intermediate resolution coverage (0.3 cm^{-1} to 5 cm^{-1}) in the 1.6 to 5.4 micron spectral interval. It has been used in the field to study radiation from aircraft exhaust plumes, background emission, and atmospheric transmission. In the laboratory, line spectra of flames have been measured and nonequilibrium vibrational temperatures derived. System configuration, operating procedure, and data processing are discussed. The performance of the interferometer is illustrated by typical spectral data.

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INTRODUCTION

The purpose of this memorandum is to illustrate the uses and capabilities of a newly acquired PFS-201 interferometer. This instrument has been used extensively in support of the OV-1D Mohawk suppressor program and has provided direct experimental verification of the suppressor performance (Ref. 1). In addition, it has been used to measure the infrared signatures of backgrounds and other aircraft. Typical results from both the field and the laboratory measurement programs are presented, and several techniques responsible for upgraded system performance are described.

The theory of interferometers is discussed extensively in the literature (Refs. 2,3,4, and 5). Briefly, an interferometer spectrometer is an instrument whose output (interferogram) is the Fourier transform of the incident wavelength spectrum. This interferogram is digitally recorded and then numerically inverted in order to recover the spectrum. The use of interferometric rather than dispersive optics allows the instrument to accept a greater amount of light (throughput or Jacquinot's advantage). The use of a Fourier transform process rather than a sequential wavelength scanning process allows all wavelengths to be measured simultaneously (multiplex or Fellgett's advantage). This mode of operation makes maximum use of the available signal and measurement time. The net result is an enhanced signal-to-noise ratio compared to conventional grating or prism spectrometers.

EXPERIMENTAL TECHNIQUE

The measurements were made with a General Dynamics model PFS-201 interferometer, (Figure 1 and Ref. 6). The capabilities of this

interferometer are significantly improved relative to an older Block model 197 used in previous work by the Grumman Research Department (Ref. 7). The main features of the instrument are summarized in Table 1. It uses a cryogenically cooled In:Sb detector to cover the 1.6 - 5.4 micron region.* The maximum resolution is 0.2 cm^{-1}, equivalent to 0.00032 micron at 4 microns. This instrument is well suited to field work. It is rugged, compact, and portable. The high optical throughput and multiplex advantage give it good sensitivity. This sensitivity is further enhanced by a six-inch Dall-Kirkham telescope that mounts onto the faceplate of the interferometer. The instrument is isolated from mechanical vibration, and an internal laser controlled servoloop maintains optical alignment of the scanning mirror. The rapid scan technique allows a complete interferogram to be measured in approximately one second. In general, successive interferograms are coadded in order to improve the signal-to-noise ratio. For time resolution of slow systems (>1 sec) successive interferograms can be examined individually. At the other extreme, a certain class of fast chemical reactions (tens of microseconds) can also be observed in great spectral detail using a repetitive pulsed photolysis technique** (Refs. 8 and 9). The interferometer has been used exclusively to generate asymmetric interferograms (single sided) because this results in a $\sqrt{2}$ improvement in signal-to-noise compared to the symmetric (double sided) case.

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* An optional modification from the manufacturer is available to extend the long wavelength response to 13 microns using a HgCdTe detector.

** In a trial run, the PFS-201 was used with a General Radio 1531 AB strobe and a sample-hold unit to produce acetone spectra with 20 microsecond time resolution and 2 cm^{-1} spectral resolution. However, the proper type of chemical flow system or nonreacting regime necessary for this technique has not yet been developed.

TABLE 1

OPTICAL AND MECHANICAL SPECIFICATIONS OF INTERFEROMETER

Detector	InSb
Wavelength Range	1.5-5.5 microns
D^*	$> 10^{11}$ (cm $Hz^{\frac{1}{2}}$/watt)
Aperture	1 in.
Telescope	6" Dall-Kirkham, f/16 optics
Optical Retardation	5 cm
Scan Velocity	0.01-3.0 cm/sec
Resolution	0.2 cm^{-1} with collimation
	1.0 cm^{-1} with foreoptics
Mirror Drive	Servocontrolled tilt, velocity, and position

The operation of the interferometer is shown schematically in Figure 2. Four aspects of this scheme deserve mention because they have significantly upgraded the accuracy and sensitivity of the instrument.

OPTICAL ALIGNMENT

The photometric accuracy of the interferometer is degraded by poor optical alignment. The instrument has a provision for alignment, which allows the tilt of the mirrors to be piezoelectrically adjusted for maximum signal. The achievement of a local maximum in signal level, however, does not guarantee that the alignment is optimum. For this, comparison with an external standard is necessary. A chopped blackbody source is observed broadband while the interferometer mirror drive is turned off, and the peak-to-peak signal amplitude is noted.

The mirror drive is then turned on, and the blackbody is observed without chopping. Now the peak-to-baseline amplitude of the interferogram is noted. For the case of perfect alignment, these two amplitudes are equal. In practice, the alignment figure of merit was found to be in excess of 95 percent.

DYNAMIC RANGE

The dynamic range in an interferogram is large - typically 100 to 1. If the gain of the tape recorder is limited by the amplitude of the interferogram peak, then the wings of the interferogram are recorded with a poor S/N ratio. This degrades the quality of high resolution spectra. Optical or electronic "chirping" provides only a limited solution to this problem. The present configuration solves the problem by recording the wings at increased gain on a second channel of the recorder. The amplifier for the second channel is compensated for electrical phase shifts from 0 to 20 kHz. This recording can be used to reconstruct a complete interferogram with an enhanced signal-to-noise ratio (equivalent 12 bits dynamic range).

SYNCHRONIZATION OF COADDED SCANS

When interferogram scans are coadded, it is important that the trigger pulse should occur at precisely the same time for each scan. Due to thermal drift (e.g., expansion of the mirrors) in the interferometer optics, however, the trigger pulse drifts slightly with time. This can cause a dramatic increase in the noise level of the spectral data. The present configuration uses a Tektronix 161-162 delayed pulse unit to cancel the effect of this drift.

LARGE DATA ARRAYS

The sheer size of high resolution interferograms (measured in tens of thousands of points) creates data handling problems.

In particular, the data can exceed the computing core space allocated to a user. This problem has been circumvented by implementing a technique due to Buijs (Ref. 10) which allows the interferogram to be processed in several pieces.

RESULTS

The various aircraft spectra shown in Figures 3 through 7 were obtained with the aircraft fixed on the ground and at extended range, so that strong atmospheric absorption was present. The interferometer was used with six-inch telescopic foreoptics. The observation time for each spectrum was limited to approximately 30 seconds, and in no case did it exceed 1 minute.

The infrared signature of a cool aircraft exhaust plume is shown in Figure 3 (resolution 3.7 cm^{-1}). The signature is composed of graybody continuum emission from hot parts and CO_2 emission from exhaust gases. Atmospheric absorption features due to H_2O, $^{12}CO_2$, $^{13}CO_2$, and N_2O are readily identified. The $^{13}CO_2$ band origin at 4.379 microns was used for wavelength calibration. The system noise level can be ascertained by examining the region from 3.8 to 4.1 microns, which is devoid of strong molecular absorption. Elsewhere the fine structure is principally due to atmospheric water vapor, not noise, and is repeatable from run to fun. Figure 4 shows details of a cool plume spectrum on an expanded scale.

The signature of a higher temperature plume is illustrated by Figure 5. A section of this spectrum is shown on an expanded scale in Figure 6. An atmospheric transmission spectrum is superposed for reference purposes so that plume self-absorption features may be more readily identified. (The path length of the atmospheric transmission spectrum is not equal to the target range.)

The data presented thus far were measured at intermediate spectral resolution. There are compelling reasons, however, for measurement at higher resolution. Molecular lines are typically several cm^{-1} apart. With a resolution of 1 cm^{-1} or better, therefore, it is possible to separate these individual lines from background features and then to perform detailed analyses of compositions and temperatures. Moreover, state-of-the-art research on backgrounds and targets is now concerned with spectral analysis on a line-by-line basis. The interferometer system was therefore upgraded (items 2 and 4 in the previous section) in order to obtain increased spectral resolution.

A plume emission spectrum measured at 0.5 cm^{-1} is shown in Figure 7. The effect of enhanced resolution is clearly seen in the 4.45 micron region, where well defined absorption lines of $^{13}CO_2$ occur. The accuracy of the line profiles has been improved by interpolation of the digitized spectrum at 0.125 cm^{-1} intervals (i.e., deconvolution techniques, Ref. 14).

The limiting high resolution capability (0.2 cm^{-1}) of the interferometer is illustrated by the spectrum of an acetylene-air flame (reaction zone) at a range of 2 meters (Figures 8 and 9). The spectrum was taken with an optical bandpass filter using Tescher's (Ref. 11) aliasing technique in order to reduce the number of data points by a factor of 5. Even so, the interferogram was 14336 points in length and had to be processed

piecemeal using Buijs' technique (Ref. 10). The entire spectrum is too long to reproduce here in full, so attention will be focused on two spectral regions of particular interest.

The flame spectrum is composed of emission from several bands of CO_2 (2100-2400 cm^{-1}) and CO (1900-2300 cm^{-1}). Figure 8 shows individual lines from the CO_2 ($00^0 1$-$00^0 0$) and ($01^1 1$-$01^1 0$) bands near 2350 cm^{-1}. The abrupt change in the intensity level at the band heads is indicative of the high temperature of the source. Individual lines of the ($00^0 1$-$00^0 0$) sequence are resolved as far as R80 (2391.66 cm^{-1}), where the line separation is 0.5 cm^{-1}.

Figure 9 shows the P branches of the CO hot bands near 2020 cm^{-1}. It is noteworthy that these CO lines are weak features in a much stronger spectrum dominated by CO_2 emission. This is typically the case in a remote sensing measurement, where high quality spectral data must be extracted from a larger, unwanted background signal. Lines can be identified from vibrational transitions (3-2), (2-1), and (1-0) (Refs. 12 and 13). A few lines from the (4-3) transition can be seen between 1980 and 2000 cm^{-1}. Once again, the separation of closely spaced lines confirms the high spectral resolution of the interferometer. (See, for example, the P20 (1-0) line at 2059.92 cm^{-1} and the P14 (2-1) line at 2060.34 cm^{-1}, where lines 0.42 cm^{-1} apart are resolved with one additional data point between the two peaks.) As an illustration of the use to which such data can be put, the rotational temperatures within each of the vibrational levels 1, 2, and 3 of CO have been deduced using a standard Boltzmann plot (Figure 10). It is important to note that, although the observed line shapes are somewhat distorted by the finite interferometer resolution, it is nevertheless possible to

correct for this effect and thus to obtain more accurate line strengths (Ref. 14). It is readily seen that the lowest excited level, $v = 1$, is equilibrated at the bulk flame temperature of 2700°K. The temperature of the levels $v = 2$ and 3, however, is more than 1000°K lower. This characteristic departure from thermodynamic equilibrium is well known in flames (Ref. 13).

SUMMARY

High resolution infrared spectra of aircraft and laboratory sources have been measured with a field-rated interferometer spectrometer. The instrument produced good quality spectral data despite limitations upon measurement time, target intensity, and range. High resolution work has affirmed the capability of monitoring individual molecular lines. In addition, the system sensitivity has been upgraded by improved measurement and data processing techniques.

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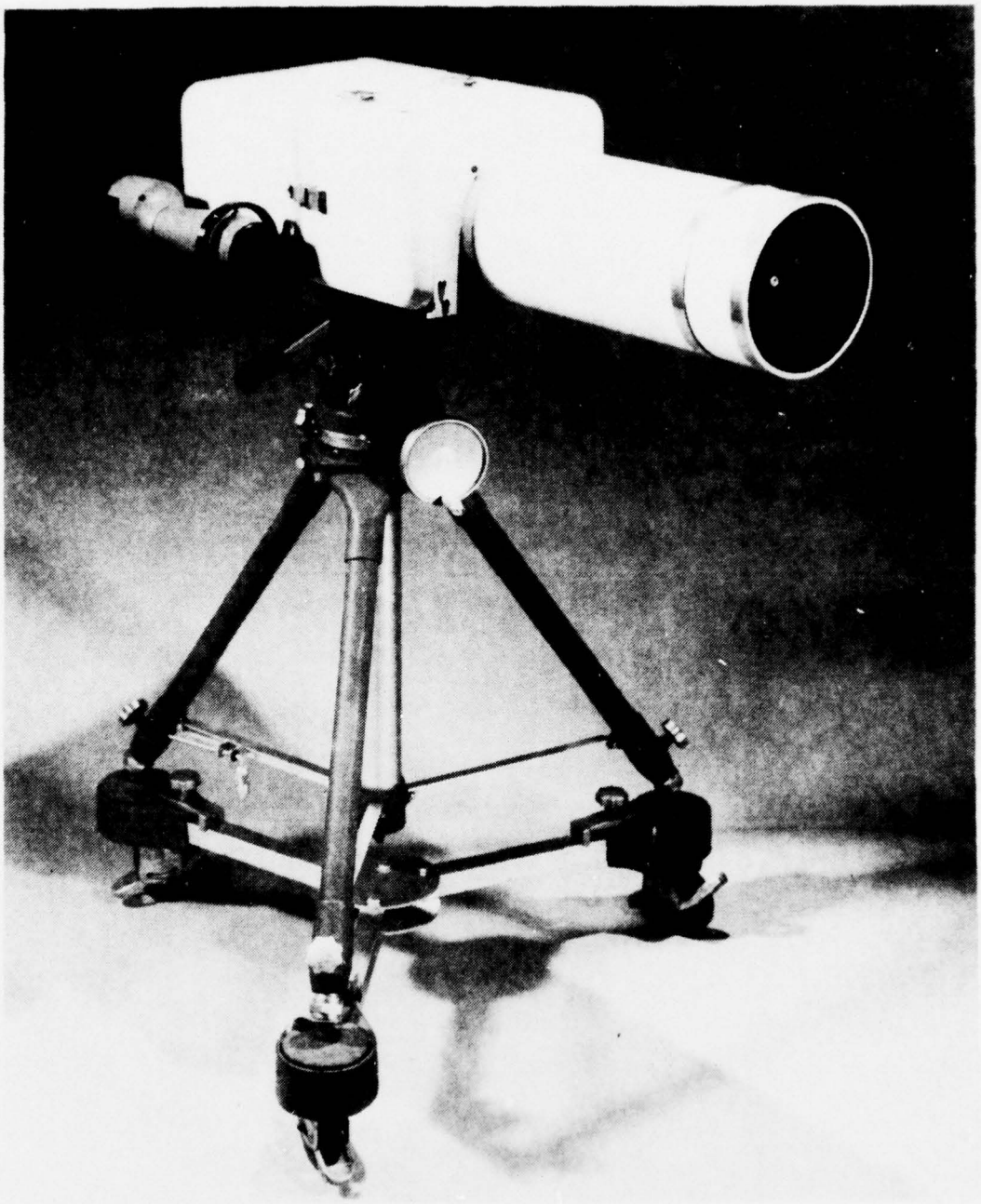

Fig. 1 THE PFS-201 INTERFEROMETER. The General Dynamics model PFS-201 interferometer is a compact tripod mounted unit designed specifically for field work. The instrument is shown with its matched f/16 6 inch Dall-Kirkham telescope and boresighted finder. A laser controlled servo loop maintains the optical alignment.

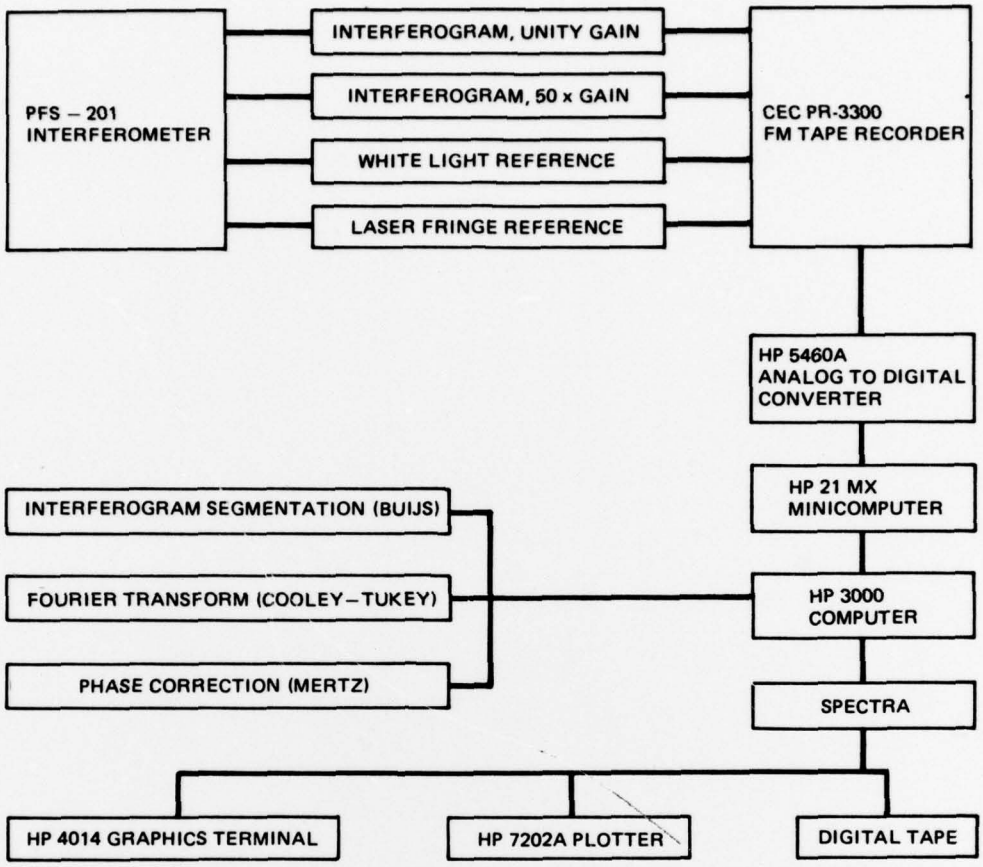

Fig. 2 OPERATION OF INTERFEROMETER. Interferometer signals are recorded on analog FM magnetic tape. The interferogram proper is recorded at two different gains in order to provide increased dynamic range. An HP 5460A A/D converter digitizes the interferogram, and an HP 21MX minicomputer coadds & stores the digital output. The coadded interferogram is transmitted to an HP 3000 computer for processing in standard high level computer languages. Interferograms exceeding the 32k core space allocated to each HP 3000 job are segmented and processed piece-wise using an algorithm devised by Buijs. The present data reduction scheme employs a complex (i.e. sine & cosine) fast Fourier transform and Mertz' phase correction technique. Spectral output is available from an HP 4014 graphics terminal, an HP 7202A plotter, or can be stored on digital magnetic tape.

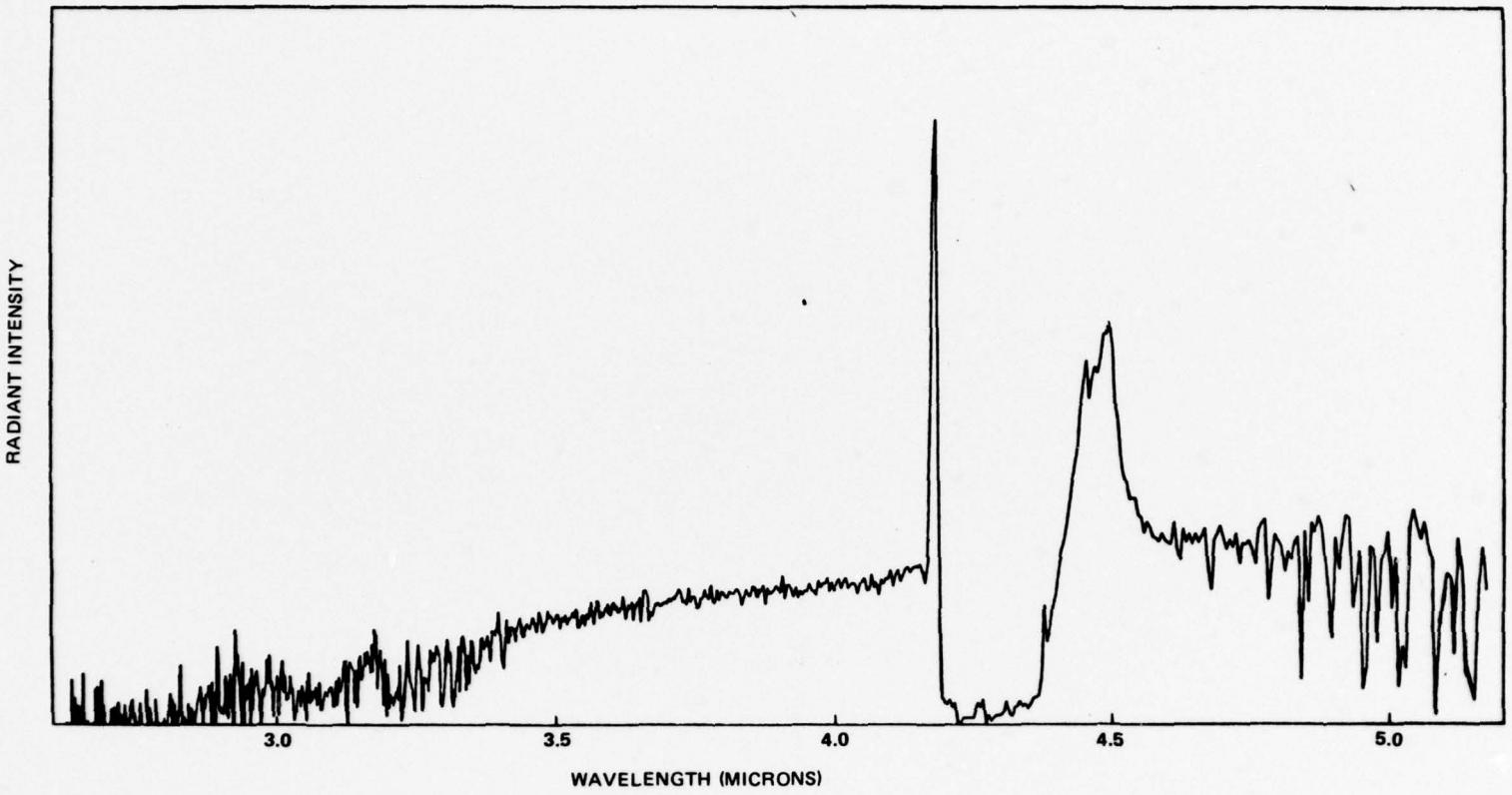

Fig. 3 SPECTRUM OF A COOL AIRCRAFT EXHAUST PLUME. The infrared signature of a cool aircraft exhaust plume is shown at a resolution of 2.7 wavenumbers. Plume emission can be seen at 4.18 and 4.5 microns. The graybody continuum emission is due to hot metal parts on the aircraft. Atmospheric water vapor is responsible for the line structure below 3.5 microns and above 4.7 microns. N_2O absorbs at 4.5 microns, and the band origin of $^{13}CO_2$ can be seen at 4.38 microns.

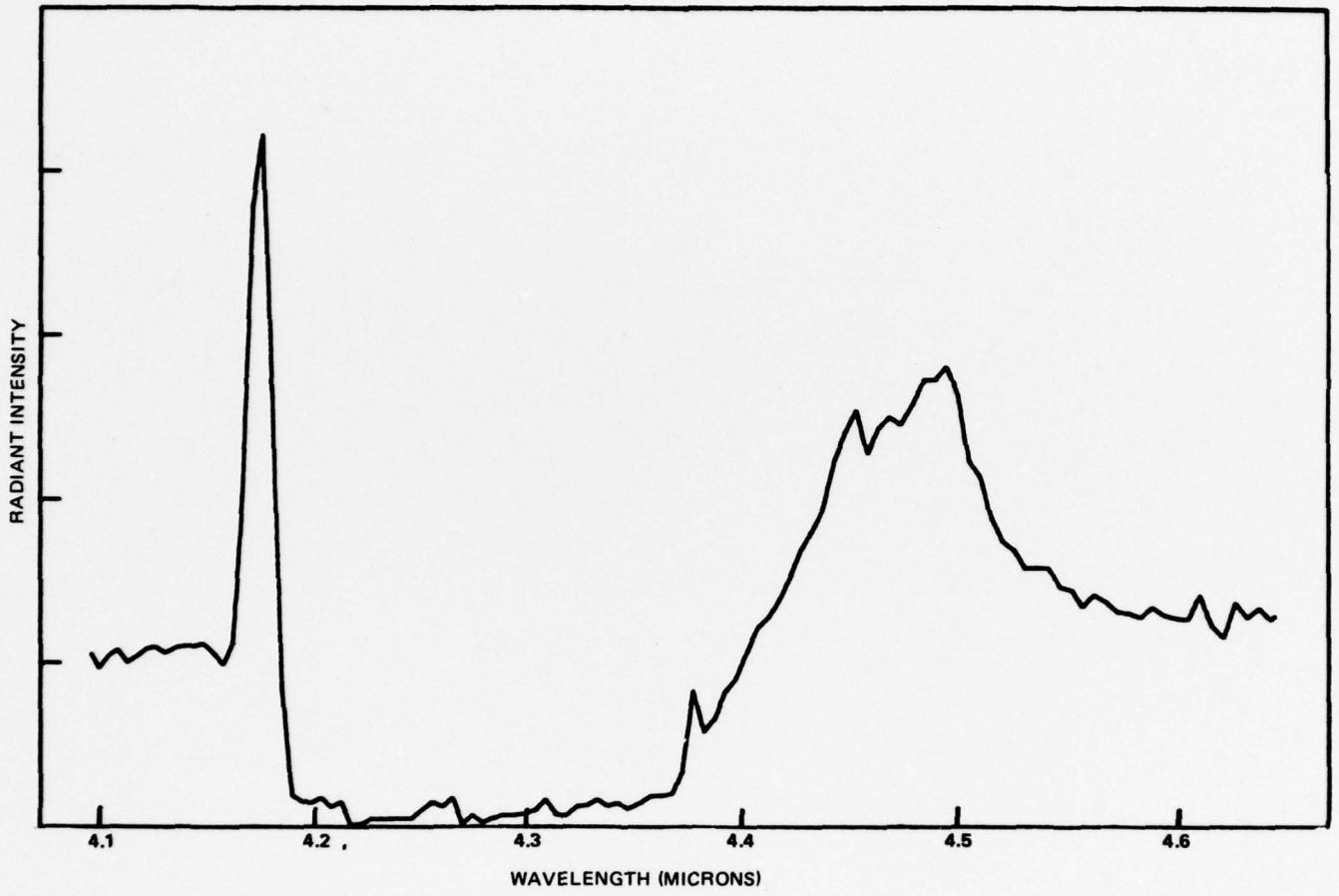

Fig. 4 SPECTRUM OF A COOL AIRCRAFT EXHAUST PLUME: EXPANDED SCALE. The signature of a cool aircraft exhaust plume is shown on an expanded scale in the region of the CO_2 4.3 micron fundamental. The spectral features are the combined result of plume emission and atmospheric attenuation.

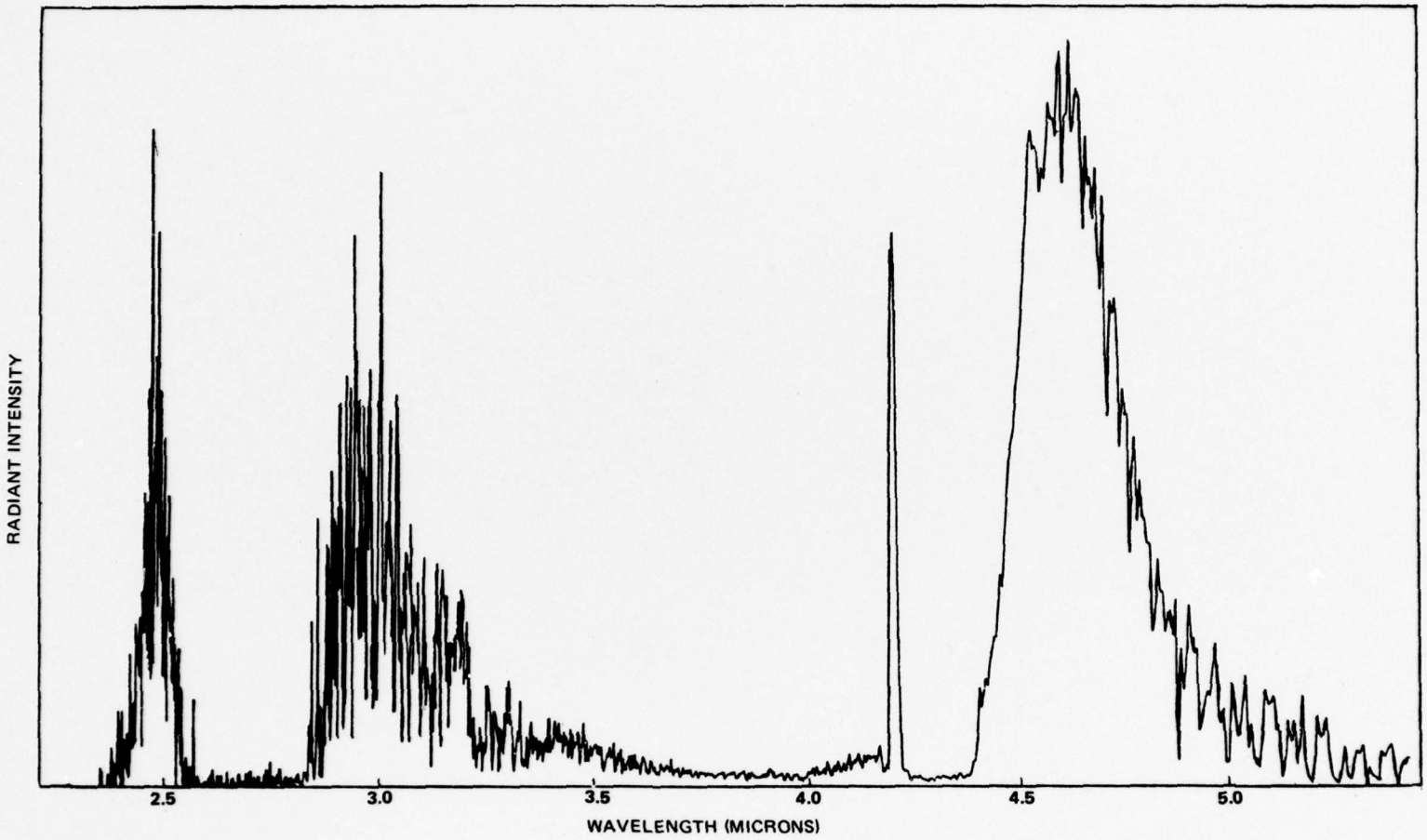

Fig. 5 SPECTRUM OF HOT AIRCRAFT EXHAUST PLUME. The infrared spectrum of a hot aircraft exhaust plume is shown at a resolution of 2.7 wavenumbers. The thermal population of H_2O and CO_2 hot bands leads to significant changes in the infrared signature compared to cooler plumes. The most noteable of these changes is the appearance of strong emission features in the wings of the 2.7 micron H_2O band.

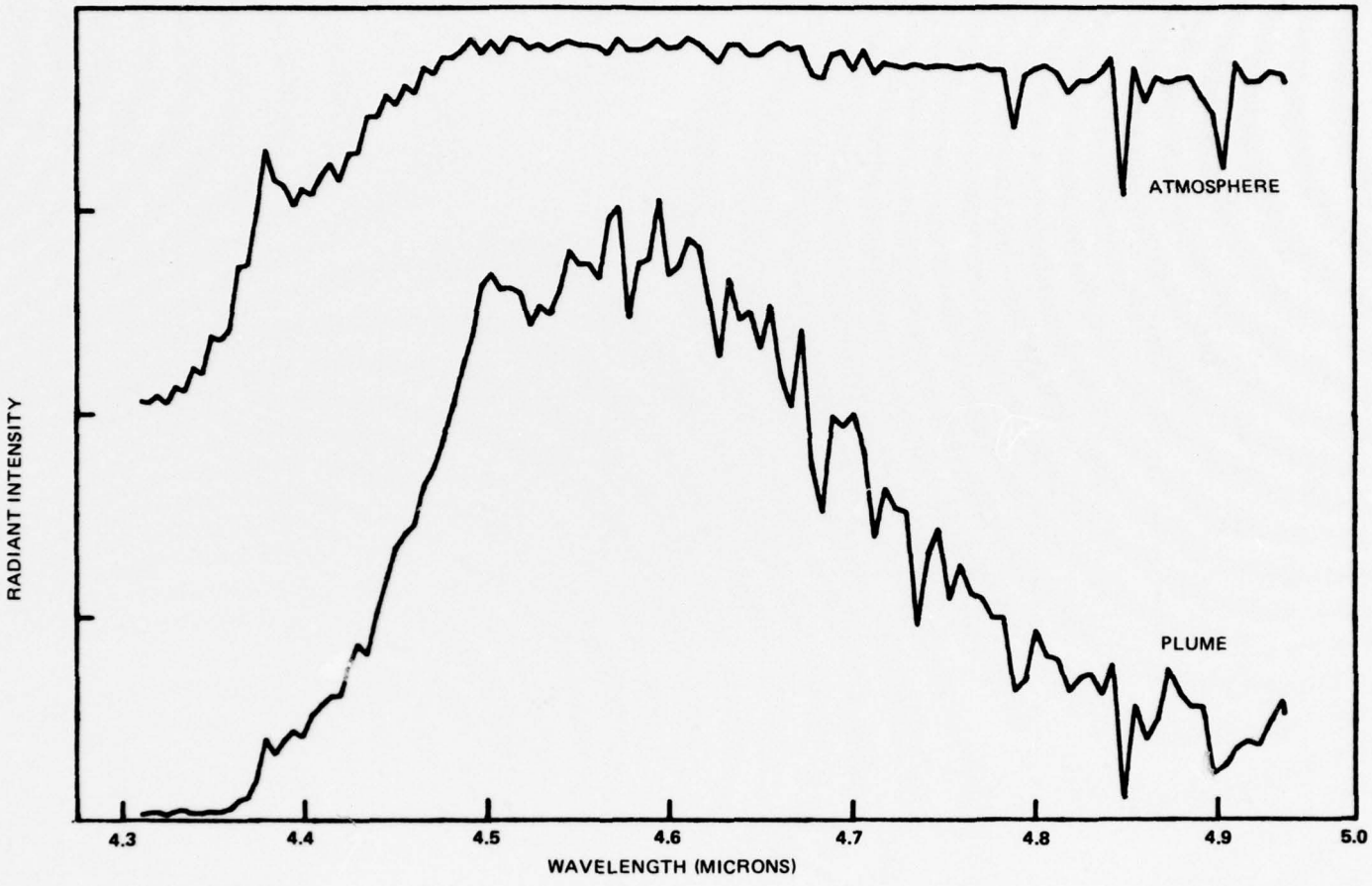

Fig. 6 SPECTRUM OF A HOT AIRCRAFT EXHAUST PLUME: EXPANDED SCALE. The region from 4.4 microns to 4.9 microns shows emission from CO_2, absorption by CO_2 and isotopic $^{13}CO_2$, absorption by atmospheric water vapor, and a large amount of self absorption within the plume itself.

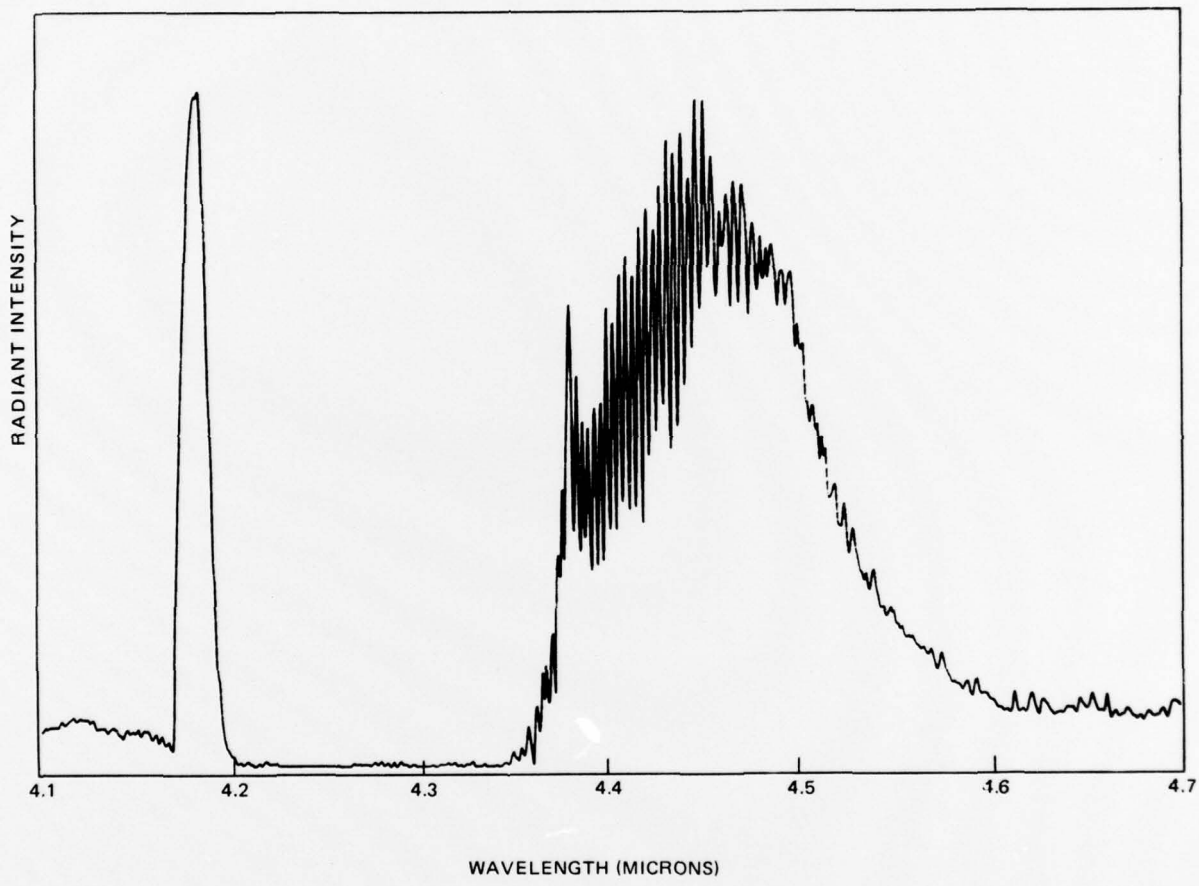

Fig. 7 Spectrum of a Cool Aircraft Exhaust Plume: High Resolution (0.5 cm^{-1}). The effect of enhanced resolution is clearly seen in this plume signature, where well defined absorption lines of atmospheric $^{13}CO_2$ can be seen. The accuracy of the line profiles has been further improved by interpolation of the digitized spectrum at 0.125 cm^{-1} intervals.

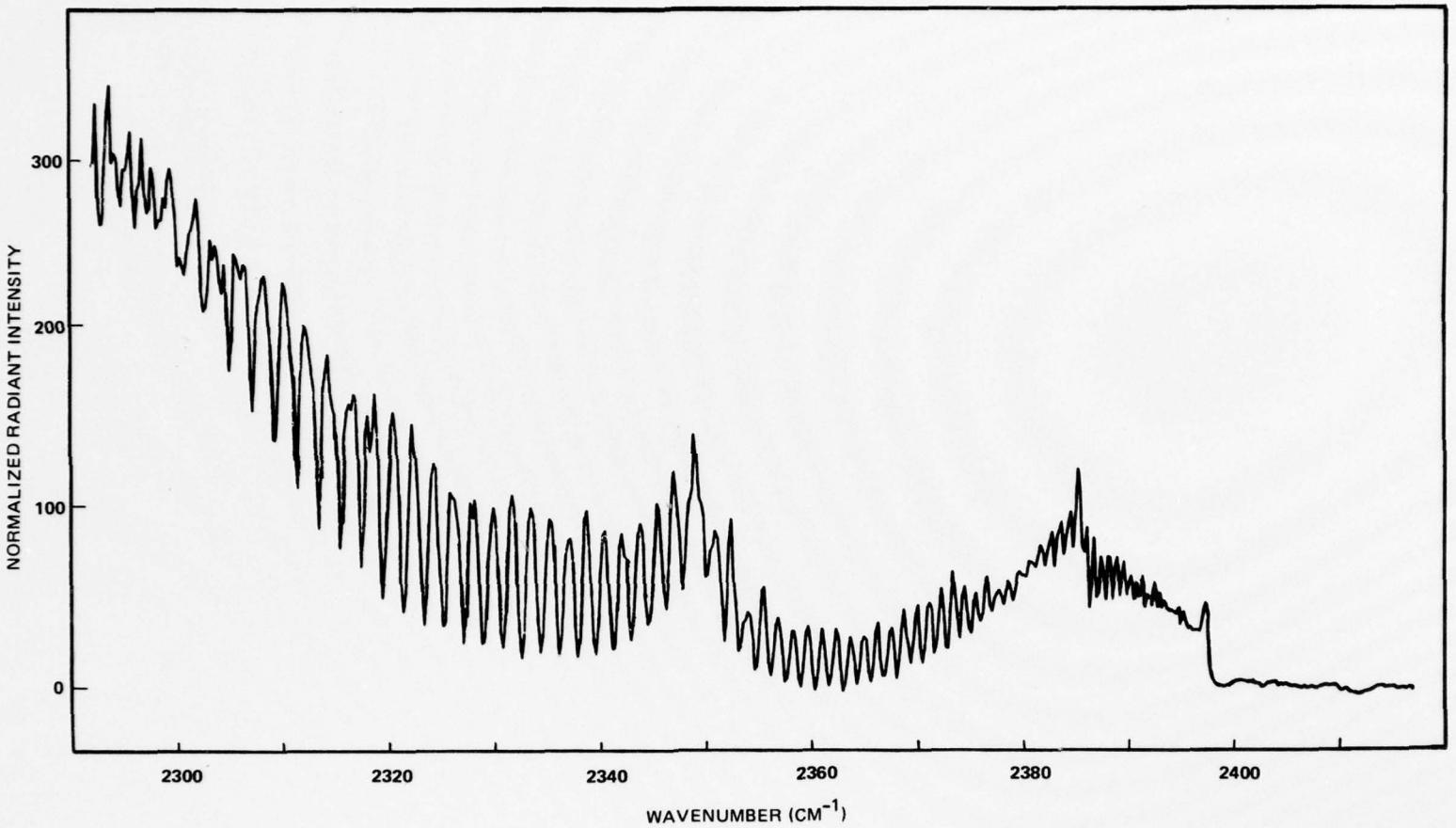

Fig. 8 SPECTRUM OF AN ACETYLENE – AIR FLAME NEAR 4.3 MICRONS. The emission from an acetylene-air flame is shown at high resolution (0.2 wavenumber) and short atmospheric path length (2 meters). The spectrum shows the regular spacing of rotational lines within the CO_2 ν_3 band. Atmospheric absorption dominates below 2380 wavenumbers and flame emission dominates above. The high temperature of the emitting gas is evident from the sharp band heads at 2385.9 wavenumbers (01'1-01'0) and 2397.5 wavenumbers ($00^\circ1$-$00^\circ0$). The ($00^\circ1$-00°) band origin can be seen at 2349.1 wavenumbers. Individual rotational lines in this band are resolved up to R80 (2391.7 cm^{-1}), where the line spacing is 0.5 cm^{-1}.

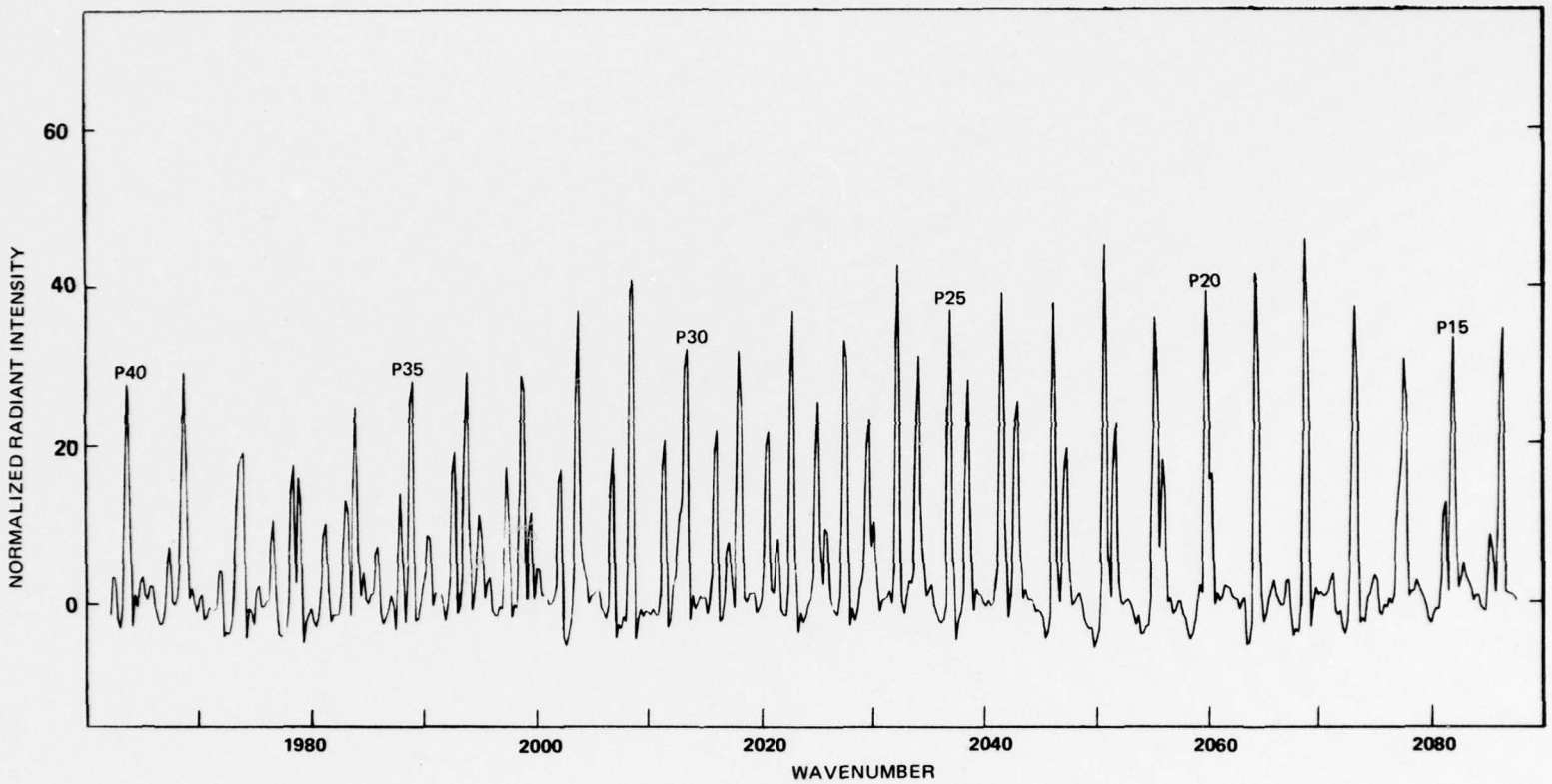

Fig. 9 SPECTRUM OF AN ACETYLENE – AIR FLAME NEAR 5.0 MICRONS. The CO emission from an acetylene-air flame can be seen near 5 microns (P branch of the 4.7 micron fundamental). The spectrum can be resolved into three periodic components from the (1-0) (2,1), and (3-2) transitions, each with a line spacing of approximately 2.8 wavenumbers. Every fifth (1-0) line is identified in the plot. The (2-1) line sequence can be most easily traced out by starting at 2060 wavenumbers and working to the left. 3-2 lines appear near 2030 wavenumbers, and weak 4-3 lines can be seen between 1980 and 2000 wavenumbers. The considerable line overlap between these bands provides a test of the instrumental resolving power.

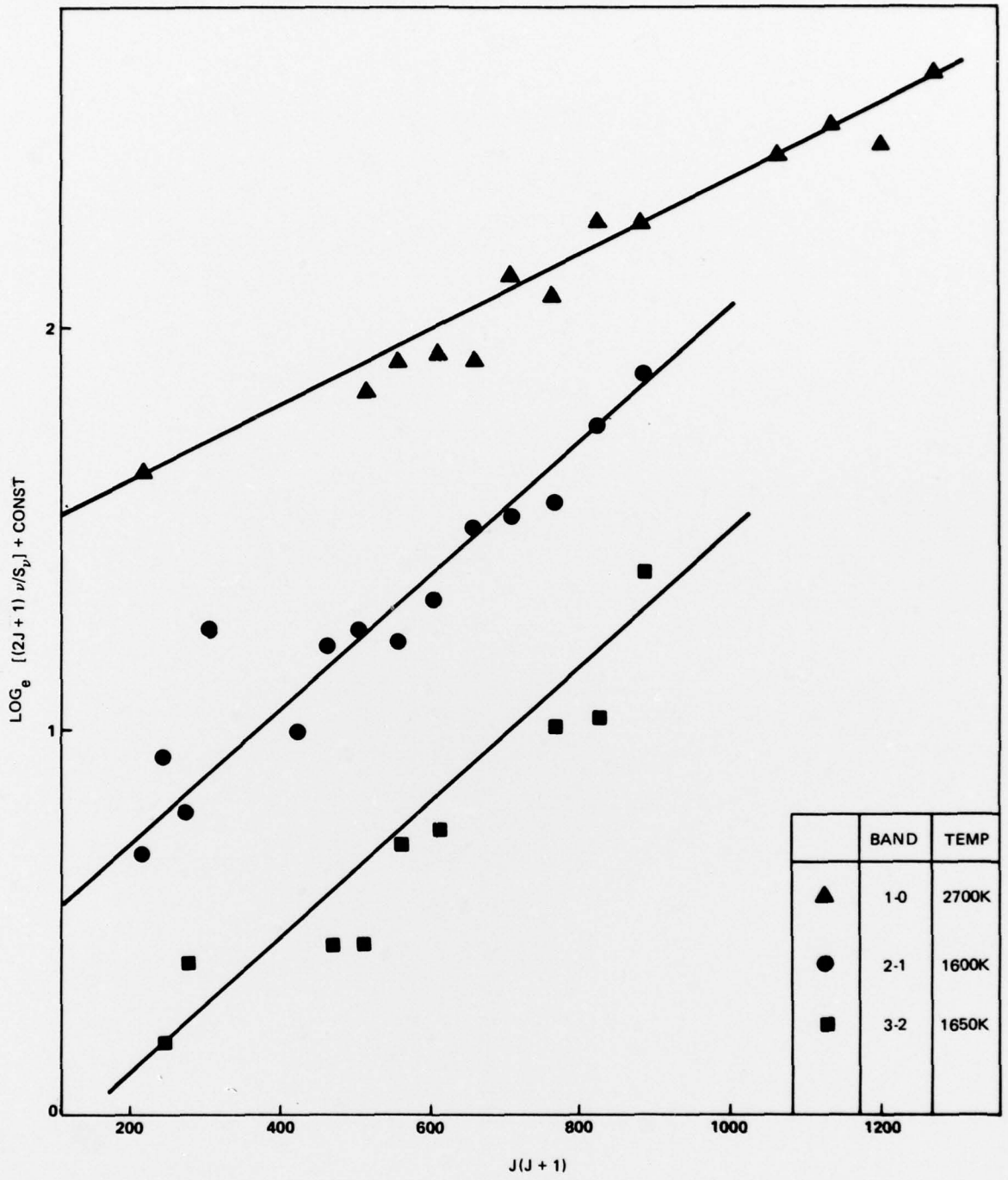

Fig. 10 DETERMINATION OF GAS TEMPERATURES USING HIGH RESOLUTION INTERFEROMETER MEASUREMENTS. Temperatures are determined spectroscopically by measuring the population ratios of different molecular states. The plot does this for the rotational J levels of three CO vibration states, ν = 1, 2, and 3. Temperature is derived from the slope of the plot. Although each vibrational manifold follows a Boltzmann distribution, the overall distribution is markedly non-equilibrium. This behavior is characteristic of flames.